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| APPLICATION NO. | FILING DATE | FIRST NAMED INVENTOR | ATTORNEY DOCKET NO. | CONFIRMATION NO. |
|---|---|---|---|---|
| 09/502,133 | 02/11/2000 | Harold E. Helson | 103544.127 | 4787 |

7590 01/25/2008

Jason A. Reyes
Hale and Dorr LLP
60 State Street
Boston, MA 02109

| EXAMINER | |
|---|---|
| JONES, HUGH M | |

| ART UNIT | PAPER NUMBER |
|---|---|
| 2128 | |

| MAIL DATE | DELIVERY MODE |
|---|---|
| 01/25/2008 | PAPER |

**Please find below and/or attached an Office communication concerning this application or proceeding.**

The time period for reply, if any, is set in the attached communication.

| Office Action Summary | Application No. | Applicant(s) |
|---|---|---|
| | 09/502,133 | HELSON, HAROLD E. |
| | Examiner | Art Unit |
| | Hugh Jones | 2128 |

*-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --*

**Period for Reply**

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

**Status**

1)☒ Responsive to communication(s) filed on *29 October 2007*.

2a)☐ This action is **FINAL**. 2b)☒ This action is non-final.

3)☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

**Disposition of Claims**

4)☒ Claim(s) *1-35* is/are pending in the application.

4a) Of the above claim(s) *2-4,6-8 and 10-12* is/are withdrawn from consideration.

5)☐ Claim(s) _____ is/are allowed.

6)☒ Claim(s) *1, 5, 9, 13-35* is/are rejected.

7)☐ Claim(s) _____ is/are objected to.

8)☐ Claim(s) _____ are subject to restriction and/or election requirement.

**Application Papers**

9)☐ The specification is objected to by the Examiner.

10)☒ The drawing(s) filed on *11 February 2000* is/are: a)☒ accepted or b)☐ objected to by the Examiner.

Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).

Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).

11)☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

**Priority under 35 U.S.C. § 119**

12)☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).

a)☐ All b)☐ Some * c)☐ None of:

1.☐ Certified copies of the priority documents have been received.

2.☐ Certified copies of the priority documents have been received in Application No. _____.

3.☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

**Attachment(s)**

1) ☐ Notice of References Cited (PTO-892)
2) ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
3) ☐ Information Disclosure Statement(s) (PTO/SB/08) Paper No(s)/Mail Date _____.
4) ☐ Interview Summary (PTO-413) Paper No(s)/Mail Date. _____.
5) ☐ Notice of Informal Patent Application
6) ☐ Other: _____.

## DETAILED ACTION

1. Claims 1, 5, 9, 13-35 of U. S. Patent 09/502,133 are in front of the office for consideration and remain pending. Claims 2-4, 6-8, 10-12 are withdrawn.

## ***Claim Rejections - 35 USC § 102***

2. The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

> A person shall be entitled to a patent unless –
>
> (b) the invention was patented or described in a printed publication in this or a foreign country or in public use or on sale in this country, more than one year prior to the date of application for patent in the United States.

3. Claims 1, 5, 9, 13-35 are rejected under 35 U.S.C. 102(b) as being clearly anticipated by Helson (The inventor's PhD thesis - of record).

4. Helson discloses:

identifying, from a connection table for a chemical structure, an instance of chemical structural symmetry in the chemical structure (pp, 145-149; fig. 4.5; chapter 4; fig. 3.5, pg. 221, fig. 4.9, fig. 5.4);

wherein the instance of symmetry includes symmetrically equivalent atoms and bonds (page 246; fig. 4.5; chapter 4, fig. 4.9, 5.4);

positioning symmetrically equivalent atoms and bonds in the chemical structure diagram in accordance with the identified symmetry (pp. 145-149; page 246; fig. 4.5; chapter 3).

Note page 203-211 (redrawing)

Table 3.1. Criteria for Aef_Redraw

| Criterion | Weight* | Description |
|---|---|---|
| 1 | 12 | Bond overlap |
| 2 | 3 | Bond alignment |
| 3 | 2 | Angle alignment |
| 4 | 8 | Bond distribution |
| 5 | 4 | Alignment and zigzag of chains |
| 6 | 2 | Alignment of ring bonds |
| 7 | 4 | Macroorientation of ring systems |
| 8 | 6 | Symmetry |
| 9 | 8 | Uniform bond length |
| 10 | 12 | Atom crowding |

*When a criterion is not applicable to a molecule its weight is set to zero. Similarly, the weights for criteria 5, 6 and 7 are adjusted to reflect the importance of the criterion to the molecule at hand.

And (pg. 149):

Algorithm 3.1. Redraw algorithm

1) Preliminary. Record preexisting stereochemistry, directions of chain bends; calculate atoms' drawing priorities, *etc.*
2) Loop on molecules present
   a) Calculate ÆF of original.
   b) Assign a drawing strategy for every ring.
   c) Choose the Head Atom and initialize work queue.
   d) Dequeue an atom (FringeAt). Is it in a ring?
      Yes:
3) Ring processing
   a) Decide which neighbor of FringeAt to place next.
   b) Decide angle at which to place neighbor.
   c) Note if there is atom crowding.
   d) If neighbor is in an undrawn ring, draw ring.
   e) Steps 3a-d are repeated until all neighbors have been placed. Then double bond stereochemistry is checked and rectified if necessary if FringeAt is in a double bond.
      No:
4) Non-ring processing. Calculate Ang_Inc, the angular distance between substituents. Place substituents accordingly, noting if atom crowding results.
5) If atom crowding was noted, invoke the anti-overlap procedure. Return to step 2d if the queue is not empty.
6) Post-placement processing
   a) Restore sense of molecule if it has been flipped.
   b) Rectify double bond stereochemistry in undrawable rings and templates.
   c) Restore $sp^3$ stereochemistry.
   d) Align molecule and its bonds with coordinate axes.
   e) Reinstate original form if ÆF has declined.
7) Reposition

5. Note that the redraw algorithm *always* calls the **reposition algorithm**. See page 145-146:

**Implementation in CAMEO**

In CAMEO, SDG is divided into two independent processes: SDG proper, referred to as "redrawing," and positioning of the resulting molecules, called "repositioning." Both facilities exist as independent packages of routines that may be called to serve different occasions; they are not rigidly tied to any particular phase of the program. In fact, repositioning does not even require perception, although redrawing does. The two executive

145

routines are REDRAW for SDG proper, and ANA_REPO for positioning. At present REDRAW, which always invokes ANA_REPO at its end, is called from the following places:

Also see the table of contents:

v

Page

CHAPTER 3. STRUCTURE DIAGRAMS FROM CONNECTION TABLES ..... 126

Abstract ..... 126
Introduction ..... 126
Purpose and Context of SDG ..... 127
Challenges to an SDG Algorithm ..... 130
Complex Ring Systems ..... 130
Special Morphologies ..... 133
Atom and Bond Overlap ..... 136
Precedents ..... 138
STR3 (1973) ..... 138
Carhart (1976) ..... 140
CAS (1977) ..... 142
Spektren (1982) ..... 143
Shelley (1983) ..... 143
University of Hull (1990) ..... 144
DEPICT (1990) ..... 144
Implementation in CAMEO ..... 145
Redraw Algorithm ..... 148
Outline ..... 148
Simple Ring Drawing and the Irregular Polygon Method ..... 156
Complex Monocyclic Rings ..... 160
Bicyclic Ring Systems ..... 163
Avoiding Congestion: Atom Priority, the Fleeing Heuristic, and the Congestion Function ..... 164
Removal of Atom and Bond Overlap and Crowding (the RBS Heuristic) ..... 167
Reposition Algorithm ..... 173
Analytic Repositioning Algorithm ..... 175
Dynamic Repositioning Algorithm ..... 185
The Jumping Heuristic ..... 194
Æsthetic Functions and the Testing Database ..... 200
AeP_Repo: æsthetic Function for Positioning Molecules ..... 202
Aef_Redraw: Æsthetic Function for Redrawing ..... 203
The Testing Database ..... 211

Page

A Unified Repositioning Algorithm ..... 228
Acknowledgement ..... 230
References and Notes ..... 231

CHAPTER 4. DETECTION OF SYMMETRY AND DUPLICATE PRODUCTS ..... 233

The need for Symmetry Perception and Identical Structure Identification ..... 233
Symmetry ..... 234
Identical Products ..... 234
Which Symmetry is Required? ..... 237
Approaches to Isomorphism and Automorphism ..... 239
Approaches to Isomorphism ..... 241
Path-Growing Yields Symmetry as well as Isomorphism ..... 242
Morgan Algorithm ..... 243
Approaches to Symmetry ..... 245
Placement in CAMEO ..... 246
Goals of Symmetry Perception in CAMEO ..... 249
Implementation of Symmetry Perception in CAMEO ..... 252

6. As for dependent claims, see pp. 169, 155-156, 173-212 (redrawing), 207-209, 227-230 (redrawing), table 4.3 (example of candidates); chapter 3 (redrawing) chapter 4 (examples of symmetry).

7. Also see:

Page xix:

| | | |
|---|---|---|
| ISI | sym | Identification of Identical Structures |
| IVP | sym | Iterative Vertex Partitioning |
| MA | sym | Morgan algorithm |
| RSCT | SDG | Ring Symmetry Conversion Table |
| SDCO | sym | Symmetry-derived canonical order |
| SDG | SDG | Structure Diagram Generation (*q.v.*) |
| SP | sym | Symmetry Perception |
| SRAB | sym | Symmetry-Reduced A/B |

page xxii:

*Connection Table* The different connection tables used by CAMEO are:

a) CSS. The ordinary structure storage format. Consists of a list of atoms, with coordinates, element type and charge, and bonds, with the atom pair forming the bond, order, and stereochemistry.
b) CNAB. During translation of a chemical name (see Graphics chpt.) a simplified, compact CT is built up. Its principal omission is atom coordinates.
c) Morgan Table. The Morgan table is a data structure similar to that used in the MA. It is used during the search for the canonical table.
d) Canonical Connection Table (CCT). A highly encoded data structure similar to the Morgan Table in which the structures' A/B's have been canonically sequenced. It is possible to tell if two structures are identical or not by comparing their CCT's.

page xxvi:

*Perception* The process in which the A/B of a structure is examined to deduce higher level information, such as the presence and location of different element types (oxygen, silicon, *etc.*), rings, aromaticity, stereochemistry, symmetry, and the *canonical connection table.*

*Perception-Derived Structure* See *Derived Structure*

*Perception Phase* (Graphics) There are five distinct occasions when perception is performed: 1) sketch-time; 2) other graphics-time; 3) pre-mechanistic; 4) mechanistic; 5) post-mechanistic. All perception is channeled through one of two executives, PERCEP (pre- and post-mechanistic) and MCHPRCP (all others). Several flags control what sort of perception-induced alterations are permissible.

page xxvii

*Reposition* (SDG) The final stage in *Structure Diagram Generation*, in which molecules are translated (shifted) to maximize the distance between them while maintaining their size as much as possible. Consists of two steps:

a) Analytic placement.
b) Dynamic repositioning. The *fragments* are treated as if they were charged particles that repel one another. They are allowed to move under each other's forces until they come to rest at equilibrium.

page xxviii

*Stereochemistry* Most important stereochemistry of organic molecules can be represented in CAMEO, *i.e.* enantiomers and double bond stereoisomers. The notable omission is allene stereochemistry. A racemic mixture is represented by the absence of wedged or dotted bonds. Mixtures of *cis*/*trans* isomers are represented by labeling the double bond with a "U"; see Appendix B for a discussion. On rare occasions, usually in bridged ring systems, the program is unable to design a diagram in which a double bond has the correct *cis* or *trans* substituent pattern; an "I" is drawn beside such bonds to indicate that their stereochemistry is opposite that shown.

*Structure* One or more molecules that collectively constitute a chemical system undergoing reaction or emerging from reaction. The structure is a unit of storage; it is described by an A/B table, a tree node number, and more or less information about its role as a starting material and/or product.

*Structure Diagram Generation* (SDG) The introduction or optimization of the two-dimensional coordinates in a connection table, especially for the purpose of realizing an aesthetic drawing. Consists of: a) Regularizing bond lengths and angles, and rendering rings in a conventional orientation. b) Redistributing molecules within the plotting area. Cf. *Reposition*.

*Symmetry* An object is symmetric if it contains components that are equivalent by some specified criteria. Equivalent components belong to the same "equivalence class," or "orbit." Frequently there are several orbits in one molecule, *e.g.* the two in butane.

Of the several types of chemical symmetry known, the one that reflects equivalent chemical reactivity is configurational symmetry.

*Symmetry-Reduced A/B (SRAB)* (Symmetry) The smallest subset of the A/B sufficient to reproduce the chemistry of the parent. In cyclohexane, for example, any one atom (bond) is representative of the entire molecule. Limiting attention to the SRAB saves computation time and avoids duplicate products due to symmetry. Reactions which involve more than one atom (bond), however, such as periodate oxidation of vicinal diols, may not rely upon the SRAB.

As has been seen, some approaches to isomorphism also yield symmetry, and vice versa. There is a fundamental reason why the two problems are related: a simple proof shows that they are formally equivalent; any method to solve one can be modified to solve the other.[4] On a practical level they appear similar because some solutions to both involve partitioning or growing paths, resulting in overlap of these algorithms.

## Placement in CAMEO

Before describing implementational details, it is shown how SP and ISI are situated within CAMEO. Fig. 4.4 highlights the overall program flow. Symmetry perception occurs during the middle of perception (whether graphic, mechanistic, pre- or post-mechanistic). CCT-coding occurs only at the end of pre- and post-mechanistic perception, *i.e.* once for the starting material and once for each product. Reaction intermediates may be perceived during the mechanistic phase but are not ordinarily CCT-coded. Because of this arrangement SP is needed and executed much more often than CCT-coding. It therefore made sense to develop an SP procedure that was fast on its own without concern for obtaining a CCT.

The symmetry algorithm requires stereochemical perception information, and must therefore reside after the point in the perception sequence where that is derived. CCT-coding could be performed at any time afterwards, and is performed at the end of a perception pass. Record is kept of which structures have been coded, so that ISI will merely check which structures are not coded, and codes them.

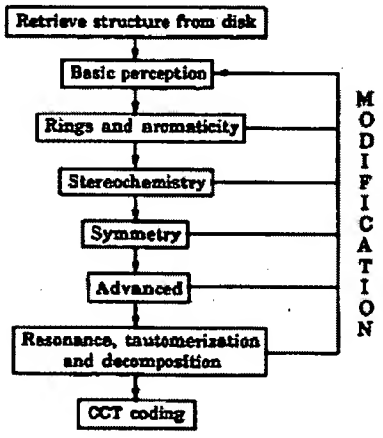



Figure 4.5. The perception phase

Page 252:

Implementation of Symmetry Perception in CAMEO

The approach we have taken to symmetry perception is entirely original, as it was conceived and implemented without benefit of the literature. Upon review of the literature it is found to be similar to that published by Shelley and Munk more than a decade earlier,[20,22] and that of Balaban *et al.* several years ago.[6,28,29] The basic strategy is Iterative Vertex Partitioning (IVP), in which local molecular irregularities are propagated through the molecule until all atoms are partitioned into a stable number of distinct types. Because our implementation was conceived independently it is somewhat different. For one thing our symmetry perception has the extra responsibilities described in the previous section. For another, Shelley and Munk's algorithm, despite its suggestions, does not know what to do with stereochemistry or aromaticity, while Balaban *et al.*'s approach cannot treat stereochemistry at all without resorting to path-growing; our method treats these features routinely and rapidly. Finally, our algorithm is the first we know of not based on path growing to yield bond symmetry as well as atom symmetry.

Fig. 4.9:

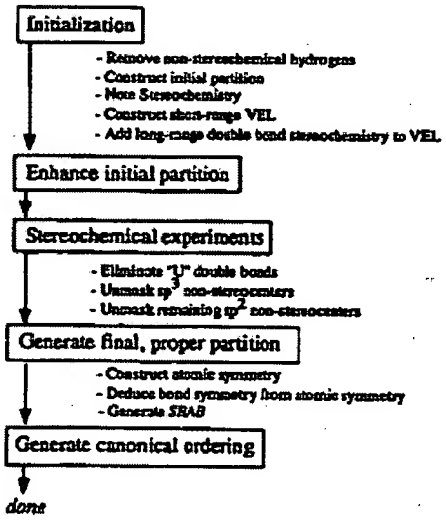



Figure 4.9. Symmetry perception

Table 4.3:

**Table 4.3. Symmetry perception timing information**

| Structure | No. Equivalence Classes: Atoms/Bonds[a] | Passes: Soft + Hard[b] | CPU[c] ($10^{-2}$sec) |
|---|---|---|---|
| methane | 1 / 0 | 0 + 0 | 0.1 |
| ethane | 1 / 1 | 1 + 1 | 0.3 |
| propane | 2 / 1 | 1 + 1 | 0.4 |
| butane | 2 / 2 | 1 + 1 | 0.7 |
| decane | 5 / 5 | 4 + 1 | 2.4 |
| decanol | 11 /10 | 4 + 0 | 1.9 |
| 2-cyanonapthalene | 12 /13 | 4 + 0 | 2.3 |
| benzopyrene | 5 / 6 | 3 + 1 | 8.3 |
| adamantane | 2 / 1 | 1 + 1 | 2.1 |
| adamantan-1-ol | 5 / 4 | 2 + 1 | 2.3 |
| adamantan-2-ol | 6 / 5 | 3 + 1 | 2.6 |
| cubane | 1 / 1 | 1 + 1 | 2.0 |
| moebius cubane | 1 / 1 | 1 + 1 | 2.0 |
| moebius cubane[d] | 1 / 2 | 7 + 3 | 6.1 |
| cubanol | 5 / 4 | 3 + 1 | 2.1 |
| benzene | 1 / 1 | 1 + 1 | 1.3 |
| naphthalene | 3 / 4 | 2 + 1 | 2.2 |
| retinol | 20 /20 | 6 + 1 | 9.3 |
| strychnine | 25 /31 | 3 + 0 | 6.4 |
| morphine | 25 /29 | 2 + 0 | 6.0 |
| muscarine | 13 /13 | 6 + 1 | 4.5 |
| isoprene | 5 / 4 | 1 + 0 | 0.5 |
| 2-methyl-2-butene | 5 / 4 | 4 + 1 | 1.3 |
| cyclohexene | 3 / 4 | 4 + 1 | 1.7 |
| 1-methylcyclohexene | 7 / 7 | 2 + 0 | 1.2 |
| 1,2-dimethyl-cyclohexene | 4 / 5 | 3 + 1 | 2.3 |
| 2,2-dimethylpropane | 2 / 1 | 1 + 1 | 0.8 |
| glycerol | 4 / 3 | 2 + 1 | 1.0 |
| penicillanic acid | 14 /15 | 5 + 1 | 4.0 |
| inositol | 18 /18 | 27 + 0 | 20.1 |
| 1-butene | 4 / 3 | 1 + 0 | 0.4 |
| *cis*-2-pentene | 5 / 4 | 2 + 0 | 0.8 |
| *t*-2-pentene | 5 / 4 | 2 + 0 | 0.9 |
| 22 as drawn | 24 /26 | 11 + 2 | 19.1 |
| racemic 22 | 18 /19 | 5 + 1 | 11.2 |
| 3-methyl-tridecane | 14 /13 | 4 + 0 | 2.8 |
| 2-methyl-tridecane | 13 /12 | 6 + 1 | 3.8 |
| 7-methyl-tridecane | 8 / 7 | 3 + 1 | 3.3 |

[a]Note that the numbers increase with decreasing symmetry. An asymmetric molecule has an equivalence class for every one of its atoms and bonds.

[b]Structures for which the number of hard passes is zero necessarily lack any (configurational) symmetry.

[c]By comparison, it took 499 sec to find the 9592 primes between 2 and 100,000, inclusive, factoring every odd number.

[d]With ring membership checks.

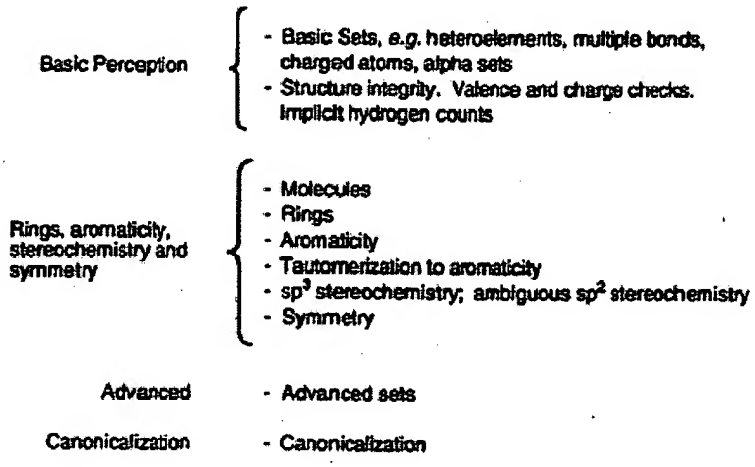



**Figure 5.4. Components of the perception phase**

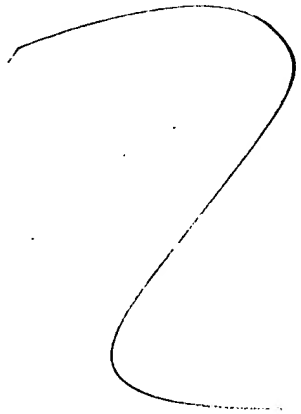
## ***Response to Arguments***

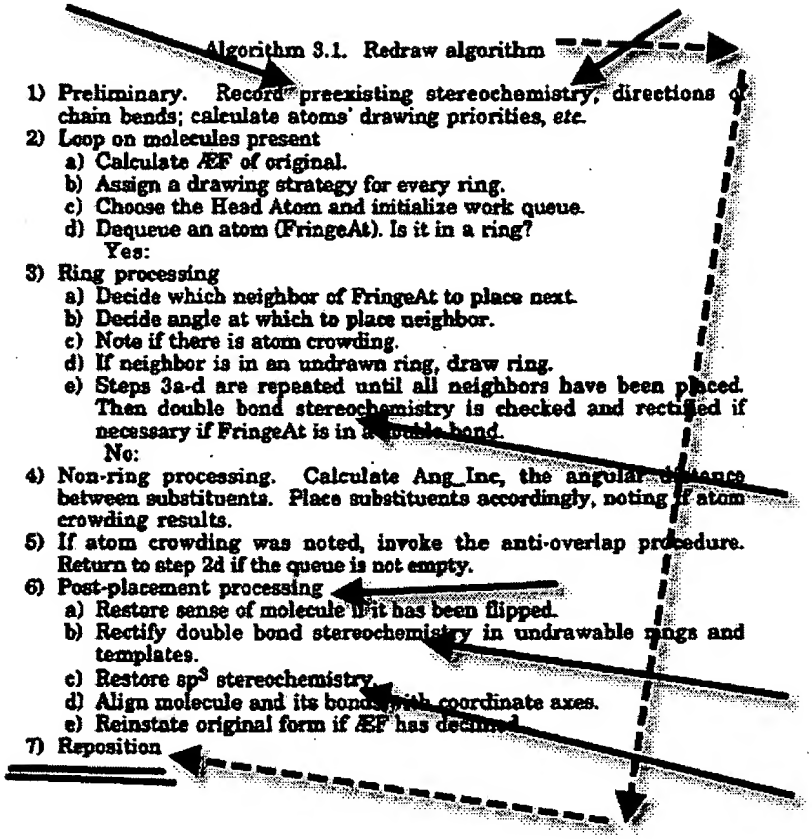
8. Applicant's arguments, filed 10/29/2007, have been carefully considered and are not persuasive. Applicants are thanked for the amendment and detailed arguments.

9. Applicant's arguments with respect to the art are not persuasive.

10. Applicants argue that the positioning and redrawing are separate and that the repositioning does not use information about the symmetry.

11, However, see "algorithm 3.1" (pg. 149):





Algorithm 3.1. Redraw algorithm

1) Preliminary. Record preexisting stereochemistry, directions of chain bends; calculate atoms' drawing priorities, *etc.*
2) Loop on molecules present
   a) Calculate ÆF of original.
   b) Assign a drawing strategy for every ring.
   c) Choose the Head Atom and initialize work queue.
   d) Dequeue an atom (FringeAt). Is it in a ring?
      Yes:
3) Ring processing
   a) Decide which neighbor of FringeAt to place next.
   b) Decide angle at which to place neighbor.
   c) Note if there is atom crowding.
   d) If neighbor is in an undrawn ring, draw ring.
   e) Steps 3a-d are repeated until all neighbors have been placed. Then double bond stereochemistry is checked and rectified if necessary if FringeAt is in a double bond.
      No:
4) Non-ring processing. Calculate Ang_Inc, the angular distance between substituents. Place substituents accordingly, noting if atom crowding results.
5) If atom crowding was noted, invoke the anti-overlap procedure. Return to step 2d if the queue is not empty.
6) Post-placement processing
   a) Restore sense of molecule if it has been flipped.
   b) Rectify double bond stereochemistry in undrawable rings and templates.
   c) Restore $sp^3$ stereochemistry.
   d) Align molecule and its bonds with coordinate axes.
   e) Reinstate original form if ÆF has declined.
7) Reposition

Note that the redraw algorithm *always* calls the **reposition algorithm**. See page 145-146:

Implementation in CAMEO

In CAMEO, SDG is divided into two independent processes: SDG proper, referred to as "redrawing," and positioning of the resulting molecules, called "repositioning." Both facilities exist as independent packages of routines that may be called to serve different occasions; they are not rigidly tied to any particular phase of the program. In fact, repositioning does not even require perception, although redrawing does. The two executive

146

routines are REDRAW for SDG proper, and ANA_REPO for positioning. At present REDRAW, which always invokes ANA_REPO at its end, is called from the following places:

12. The 103 rejections are withdrawn in order to reduce the number of issues.

*Conclusion*

**13. Any inquiry concerning this communication or earlier communications from the examiner should be:**

directed to: Dr. Hugh Jones telephone number (571) 272-3781,

Monday-Thursday 0830 to 0700 ET,

***or***

the examiner's supervisor, Kamini Shah, telephone number (571) 272-2279.

Any inquiry of a general nature or relating to the status of this application should be directed to the Group receptionist, telephone number (703) 305-3900.

**mailed to:**

Commissioner of Patents and Trademarks

Washington, D.C. 20231

**or faxed to:**

(703) 308-9051 (for formal communications intended for entry)

***or*** (703) 308-1396 (for informal or draft communications, please label *PROPOSED* or *DRAFT*).

Dr. Hugh Jones

Primary Patent Examiner

January 21, 2008

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| L2 | 1 | ("4967372").PN. | USPAT | OR | OFF | 2008/01/21 00:04 |
| L3 | 0 | symmetry and 1 | USPAT | OR | OFF | 2008/01/21 00:04 |
| L4 | 1 | symmetry and 2 | USPAT | OR | OFF | 2008/01/21 00:05 |
| L5 | 2680 | connection adj table | USPAT; EPO | OR | ON | 2008/01/21 00:06 |
| L6 | 1668 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:06 |
| L7 | 22173 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:07 |
| L8 | 3582 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:07 |
| L9 | 1 | 5 and 8 | USPAT; EPO | OR | ON | 2008/01/21 00:07 |
| L10 | 0 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:07 |
| L11 | 0 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:07 |
| L12 | 1 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:09 |
| L13 | 1 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:35 |
| L14 | 2797632 | (position$ or repositio... | USPAT; EPO | OR | ON | 2008/01/21 00:35 |
| L15 | 29 | (chemical adj3 symm... | USPAT; EPO | OR | ON | 2008/01/21 00:37 |
| L16 | 22188 | symmetry same 14 | USPAT; EPO | OR | ON | 2008/01/21 00:36 |
| L17 | 137 | chemical same 16 | USPAT; EPO | OR | ON | 2008/01/21 00:38 |
| L18 | 2 | 5 and 17 | USPAT; EPO | OR | ON | 2008/01/21 00:39 |
| L19 | 27 | mirror and 17 | USPAT; EPO | OR | ON | 2008/01/21 00:43 |
| L20 | 37 | reflection and 17 | USPAT; EPO | OR | ON | 2008/01/21 00:43 |
| L21 | 26 | 20 not 19 | USPAT; EPO | OR | ON | 2008/01/21 00:43 |